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A Social Network-Guided Approach to Machine Learning for Metal-Organic Framework Property Prediction

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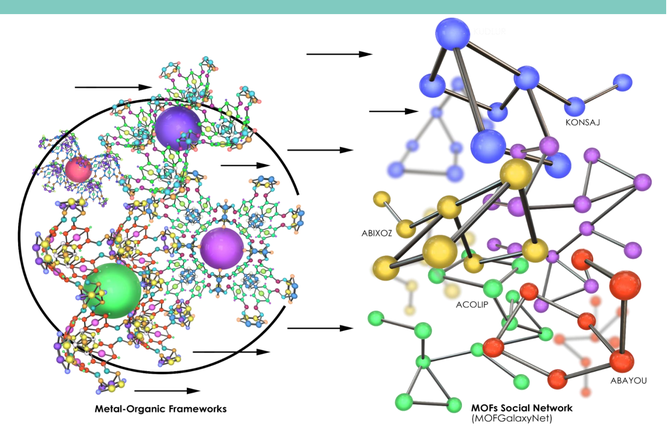
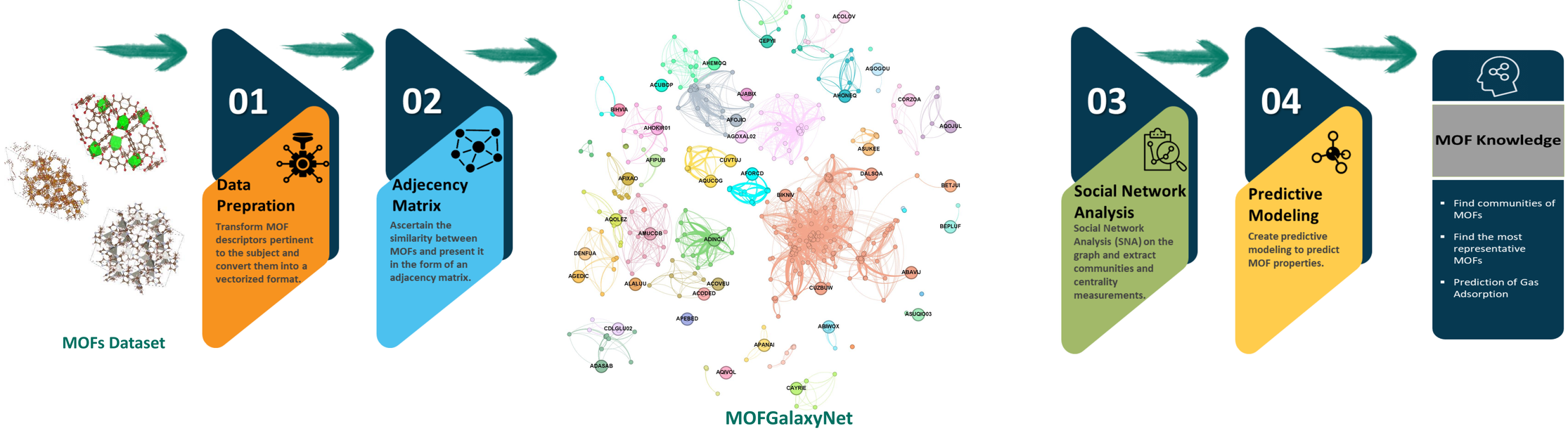
Motivation

- Reducing experimental and computational time and improving the quality of materials properties prediction is crucial when dealing with abundant research data in metal-organic framework (MOF) materials.
- Graph learning and social network analysis (SNA), an ML-based method, can be employed to analyze the materials data within a social network framework to address these challenges.
- This research aims to convert MOFs into a social network, referred to as MOFGalaxyNet, and then utilize this social network to enhance the accuracy of gas adsorption prediction. This network draws inspiration from the phenomenon of galaxies.



Method

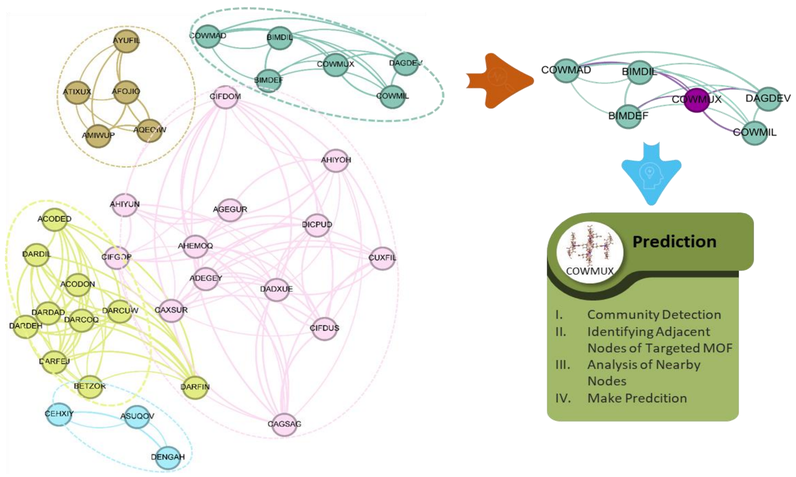
- This study created a social network, MOFGalaxyNet, using geometric descriptors obtained from the MOFs database.
- Following the development of MOFGalaxyNet, social network analytics were used in conjunction with graph-mining algorithms to extract valuable insights from the MOF data.



Experimental Results

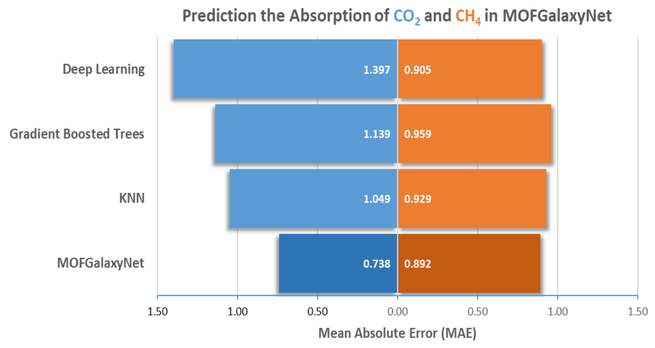
MOFGalaxyNet Communities

- Community detection refers to identifying MOF groups with similar structural and chemical characteristics.
- Considering the characteristics of neighboring MOFs in the community can predict the properties of a specific MOF.
- Community detection provides a high-throughput screening method for MOFs datasets and can detect anomalies in materials data.



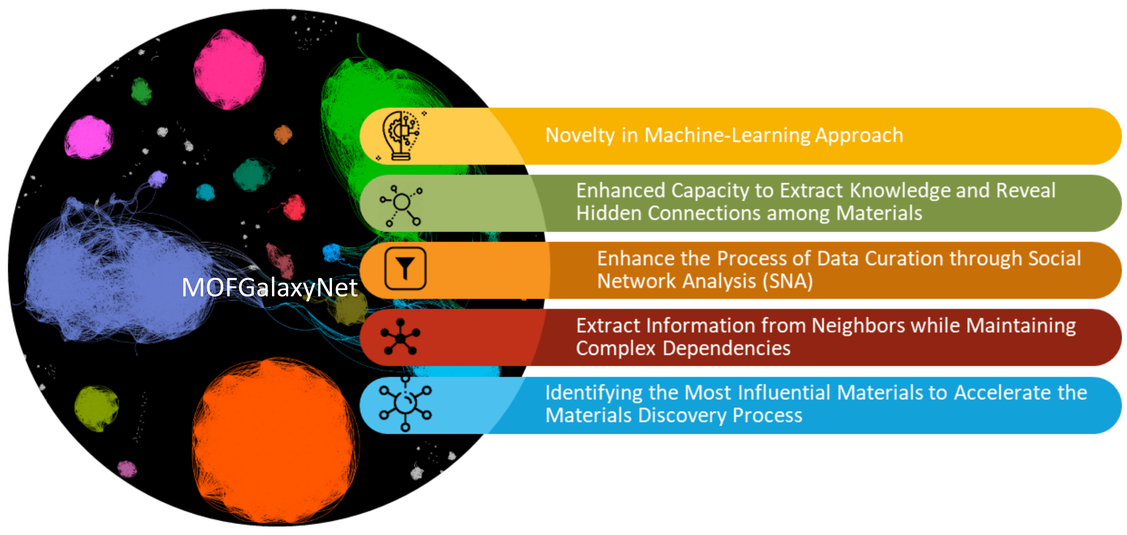
MOFGalaxyNet to Predict Gas Adsorption

- An evaluation was conducted to determine the effectiveness of using communities extracted from MOFGalaxyNet to predict MOFs' gas adsorption properties for CO2 and CH4.
- The study evaluated the effectiveness of various machine learning algorithms and compared them to MOFGalaxyNet using the mean absolute error (MAE). The results indicated that MOFGalaxyNet was more accurate than the other algorithms.



Conclusion and Future Direction

Revolutionizing Material Discovery: The Superiority of Social Network Analysis Over Conventional Machine Learning



- The suggested SNA methodology can expedite the analysis of MOF structures, even with increased theoretical and experimental data.
- The innovative MOFGalaxyNet framework can be expanded to manage vast MOF databases.
- This approach can be extended to other materials, such as high-entropy alloys (HEAs).

References and Related Published Papers

I. Jalali, M., Tsotsalas, M., & Wöll, C. (2022). MOFGalaxyNet: Exploiting Metal-Organic Framework Relationships via Social Network Analysis. Nanomaterials.

II. Ghouchan Nezhad Noor Nia, R., Jalali, M., Mail, M., Ivanisenko, Y., & Kübel, C. (2022). Machine Learning Approach to Community Detection in a High-Entropy Alloy Interaction Network. ACS omega.

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